QUANTUM THEORY OF ELECTRON TRANSPORT IN MESOSCOPIC SYSTEMS

Final Technical Report

by

Carlo Jacoboni, Antonio Abramo, Paolo Bordone, Marco Pascoli

(September 1997)

United States Army

EUROPEAN RESEARCH OFFICE OF THE U.S. ARMY

London England

CONTRACT NUMBER: N68171-96-C-9089

Istituto Nazionale per la Fisica della Materia,

Genova, Italy

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	30 September '97	FINAL AUGUST '96 -- JULY '97

4. TITLE AND SUBTITLE
Quantum theory of electron transport in mesoscopic systems

5. FUNDING NUMBERS
N68171-96-C-9089

6. AUTHOR(S)
Carlo Jacoboni, Antonio Abramo, Paolo Bordone, Marco Pascoli

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Istituto Nazionale per la Fisica della Materia
Corso Perrone 24
16152 GENOVA
Italy

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
European Research Office
Army Research Office
Office of Naval Research

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

We have developed an approach for numerical Monte Carlo solution of the Wigner transport equation for a mesoscopic system. In particular the Wigner function formalism has been used to analyze the quantum dynamics of charge carriers in presence of electron-phonon interaction in open mesoscopic systems, making use of the perturbation theory with the external fields incorporated into the unperturbed Hamiltonian. Wigner trajectories have been identified both for the ballistic propagation and for the case in which electron-phonon scattering is included. An equation for the Wigner function in a finite region inside given boundaries, using suitable boundaries conditions, has been derived. As a case of study a step potential profile has been considered. The current as a function of the step potential as obtained with the Wigner function corrected by the effect of an electron-phonon scattering process is presented. On the coherent transport standpoint, the role of the magnetic field on the condactance of wells has been investigated.

14. SUBJECT TERMS	15. NUMBER OF PAGES	16. PRICE CODE
	28	

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. Z39-18
298-102

Abstract

We have developed an approach for numerical Monte Carlo solution of the Wigner transport equation for a mesoscopic system. In particular, the Wigner function (WF) formalism has been used to analyze the quantum dynamics of charge carriers in presence of electron-phonon interaction in open mesoscopic systems making use of the perturbation theory with the external fields incorporated into the unperturbed Hamiltonian. Wigner trajectories have been identified both for the ballistic propagation and for the case in which electron-phonon scattering is included. The concept of Wigner trajectories has been used as a guiding line to face the problem of finding an equation for the WF in a finite region inside given boundaries, using suitable boundaries conditions. As a case of study a step potential profile has been considered. The current as a function of the step potential as obtained with the WF corrected by the effect of an electron-phonon scattering process is presented. On the coherent transport standpoint, the role of the magnetic field on the condactance of wells has been investigated.

Keywords: Quantum transport, Wigner function, Mesoscopic systems

Contents

I. INTRODUCTION

A rigorous quantum transport theory of electrons in semiconductor structures including both coherent propagation and scattering mechanisms is still lacking even though its need has been recognized since many years. In particular we miss a theory feasible for numerical calculations to be compared with experimental results and/or with results of the semiclassical theory with the purpose of enlightening the different predictions of the two models.

The Wigner function (WF) approach [1] provides a rigorous quantum-mechanical tool and constitues a direct link between quantum and classical descriptions of the evolution of the system in phase space. In this approach however electron-phonon (e-p) interaction has been treated using either relaxation time [2,3] or a classical Boltzmann collision operator [4]. In this work several advancements in the efford to solve the above problem exactly are presented.

The definition of the WF can be extended to include electrons interacting with phonons as follows [5]:

$$f_w\left(\boldsymbol{r},\boldsymbol{p},n_{\boldsymbol{q}},n'_{\boldsymbol{q}},t\right)=\int d\boldsymbol{r}'\,e^{-i\frac{\boldsymbol{p}}{\hbar}\cdot\boldsymbol{r}'}\rho\left(\boldsymbol{r}+\boldsymbol{r}'/2,n_{\boldsymbol{q}};\boldsymbol{r}-\boldsymbol{r}'/2,n'_{\boldsymbol{q}}\right) \tag{1}$$

where $\boldsymbol{r}$ and $\boldsymbol{p}$ are the electron position and momentum, ρ is the density matrix for the system formed by an electron and the phonon gas, and $n_{\boldsymbol{q}}$ is the occupation number of the phonon mode $\boldsymbol{q}$. Trace over the phonon variables will lead to the traditional electron WF.

In what follows we discuss an integral equation for the above WF and apply it to study quantum electron transport in open systems in presence of scattering. In particular suitable boundary conditions can be used which restrict the analysis of the WF inside a finite domain. Wigner trajectories have been identified also for the case of e-p interaction and constitute a guiding criterion for replacing initial conditions with boundary conditions for the integral equation.

Our theoretical model allows us to evaluate the correction to the WF due to the effect of an e-p scattering event.

II. THEORETICAL MODEL

A three-dimensional system of indipendent electrons interacting with phonons is considered with translational invariance along two directions (x-y). The unperturbed Hamiltonian $\mathbf{H}_\circ$ of the system contains the electron Hamiltonian, including the potential profile and the free-phonon term:

$$\mathbf{H}_\circ = \mathbf{H}_e + \mathbf{H}_p = \frac{\mathbf{p}^2}{2m} + \mathbf{V}(z) + \sum_{\boldsymbol{q}} \mathbf{a}_{\boldsymbol{q}}^\dagger \mathbf{a}_{\boldsymbol{q}} \hbar\omega_{\boldsymbol{q}} \tag{2}$$

where $\mathbf{p}$ is the electron momentum, m is the electron effective mass, $\mathbf{V}(z)$ is the electron potential profile (including the applied voltage), $\mathbf{a}_{\boldsymbol{q}}$ and $\mathbf{a}_{\boldsymbol{q}}^\dagger$ are the annihilation and creation operators of the phonon $\boldsymbol{q}$ with frequency $\omega_{\boldsymbol{q}}$. $\mathbf{H}_{e-p}$ is the e-p interaction:

$$\mathbf{H}_{e-p} = \sum_{\boldsymbol{q}} i\hbar F(\boldsymbol{q}) \left[\mathbf{a}_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} - \mathbf{a}_{\boldsymbol{q}}^\dagger e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\right] \tag{3}$$

where $F(\boldsymbol{q})$ is a function that depends on the type of e-p interaction. In the present work polar optical phonons have been considered.

The staring point of our theoretical approach is the WF generalized to include phonons in the system, in a single electron approach, as described in Eq.(1).

The time evolution of the density matrix is described by the Liouville-von Neumann equation. Starting from this equation we derived the following integral equation for the WF:

$$\begin{aligned} f_w\left(\boldsymbol{r},\boldsymbol{p},n_{\boldsymbol{q}},n'_{\boldsymbol{q}},t\right) = {} & \frac{1}{h^3}\sum_{n,n'} f_{nn'}(\boldsymbol{r},\boldsymbol{p})\, e^{-i\left(\omega(n,n_{\boldsymbol{q}})-\omega\left(n',n'_{\boldsymbol{q}}\right)\right)(t-t_\circ)} \int d\boldsymbol{r}' \int d\boldsymbol{p}'\, f^*_{nn'}(\boldsymbol{r}',\boldsymbol{p}') \\ & \times f_w\left(\boldsymbol{r}',\boldsymbol{p}',n_{\boldsymbol{q}},n'_{\boldsymbol{q}},t_\circ\right) + \frac{1}{h^3}\sum_{n,n'} f_{nn'}(\boldsymbol{r},\boldsymbol{p}) \int_{t_\circ}^{t} dt'\, e^{-i\left(\omega(n,n_{\boldsymbol{q}})-\omega\left(n',n'_{\boldsymbol{q}}\right)\right)(t-t')} \\ & \times \sum_{mm_{\boldsymbol{q}}} \int d\boldsymbol{r}' \int d\boldsymbol{p}' \left\{\mathcal{H}'(nn_{\boldsymbol{q}},mm_{\boldsymbol{q}})\, f^*_{mn'}(\boldsymbol{r}',\boldsymbol{p}')\, f_w\left(\boldsymbol{r}',\boldsymbol{p}',m_{\boldsymbol{q}},n'_{\boldsymbol{q}},t'\right)\right. \\ & \left. - f^*_{nm}(\boldsymbol{r}',\boldsymbol{p}')\, f_w(\boldsymbol{r}',\boldsymbol{p}',n_{\boldsymbol{q}},m_{\boldsymbol{q}},t')\, \mathcal{H}'\left(mm_{\boldsymbol{q}},n'n'_{\boldsymbol{q}}\right)\right\} \end{aligned} \tag{4}$$

In the above equation $\mathcal{H}' = \mathbf{H}'/i\hbar$, and $\mathcal{H}'(nn_{\boldsymbol{q}},mm_{\boldsymbol{q}})$ are its matrix elements on the basis $\{|\phi_l,n_{\boldsymbol{q}}\rangle\}$ of $\mathbf{H}_\circ$. The coefficients $f_{lm}(\boldsymbol{r},\boldsymbol{p})$ are given by

$$f_{lm}(\boldsymbol{r},\boldsymbol{p}) = \int d\boldsymbol{r}'\, e^{-i\frac{\boldsymbol{p}}{\hbar}\cdot\boldsymbol{r}'} \langle \boldsymbol{r}+\boldsymbol{r}'/2|\,\phi_l\rangle \langle \phi_m\,|\boldsymbol{r}-\boldsymbol{r}'/2\rangle \tag{5}$$

They allow to move from the WF to the density-matrix representation and viceversa. Finally $\hbar\omega(n, n_{\boldsymbol{q}})$ indicates the total unperturbed energy of the e-p system when the electron is in the n-th eigenstate and the phonon bath is in a state with n phonons in mode $\boldsymbol{q}$.

In Eq. (4) the first term in the r.h.s. describes the ballistic coherent propagation from the initial time $t_\circ$ to the observation time t. The second term describes the contribution of the unknown WF to the "last" interaction vertex at any time t' between $t_\circ$ and t followed by the free propagation from t' to t. Even though the equation is written for the entire system and contains also the phonon variables, it has been shown that a Monte Carlo solution allows for a proper average over the phonon coordinates, as long as hot-phonon effects are neglected [6].

III. WIGNER TRAJECTORIES

It is well known that a point-like electronic WF in phase space cannot represent a real physical system, since it violates the uncertainty principle. We may however consider the evolution in time of a $\delta-$like contribution to the WF $\delta^3(\boldsymbol{r}-\boldsymbol{r}_\circ)\,\delta^3(\boldsymbol{p}-\boldsymbol{p}_\circ)\,f_P\left(n_{\boldsymbol{q}}, n'_{\boldsymbol{q}}\right)$ inside Eq. (4). For free electrons its trajectory in phase space is the same as for semiclassical particles. In fact, for a plane-wave basis the coefficients f_{lm} are given by

$$f_{\boldsymbol{k}_l\boldsymbol{k}_m}(\boldsymbol{r},\boldsymbol{p}) = \hbar^3 e^{i(\boldsymbol{k}_l-\boldsymbol{k}_m)\cdot\boldsymbol{r}}\delta^3\left(\boldsymbol{p}-\hbar\frac{(\boldsymbol{k}_l+\boldsymbol{k}_m)}{2}\right) \tag{6}$$

and the ballistic evolution of the WF as given by the first term on the rhs of Eq.(4) yields [7]:

$$f_w\left(\boldsymbol{r},\boldsymbol{p},n_{\boldsymbol{q}},n'_{\boldsymbol{q}},t\right) = f_w\left(\boldsymbol{r}-\frac{\boldsymbol{p}}{m}(t-t_\circ),\boldsymbol{p},n_{\boldsymbol{q}},n'_{\boldsymbol{q}},t_\circ\right) e^{-i\left(\omega(n_{\boldsymbol{q}})-\omega\left(n'_{\boldsymbol{q}}\right)\right)(t-t_\circ)} \tag{7}$$

where m is the electron effective mass and $\hbar\omega(n_{\boldsymbol{q}})$ is the total energy of the phonon bath in the state $\{n_{\boldsymbol{q}}\}$. The first factor and the exponential factor describe the free trajectory of the electron and the time evolution of the free-phonon bath, respectively.

This result is not surprising since in absence of scattering and up to quadratic potentials (harmonic oscillator) a differential equation can be written for the WF that coincides with the Boltzmann equation, so that the dynamical evolution of the WF follows the same trajectories of the representative points of a classical gas. This implies a deformation of the WF while evolving in time due to the fact that, as time increases, the higher-momentum components move faster than the lower-momentum components.

If phonon scattering is included, similar trajectories exist, with very interesting properties, as long as a single interaction diagram is considered without time integrations. In order to prove this result let us calculate first the matrix elements of the interaction Hamiltonian $\mathcal{H}'$ in Eq. (4). Assuming a constant potential and using again plane waves as basis set, we have:

$$\begin{aligned}\mathcal{H}'\left(nn_{\boldsymbol{q}}, mm_{\boldsymbol{q}}\right) &= \left\langle \phi_n, n_{\boldsymbol{q}}\right| \mathcal{H}' \left|\phi_m, m_{\boldsymbol{q}}\right\rangle \\ &= \sum_{\sigma=1,-1} \sum_{\boldsymbol{q}} F\left(\boldsymbol{q}\right) \prod_{\boldsymbol{q}'\neq\boldsymbol{q}} \sqrt{m_{\boldsymbol{q}} + \frac{1}{2}\left(1-\sigma\right)}\, \delta_{n_{\boldsymbol{q}'} m_{\boldsymbol{q}'}} \delta_{n_{\boldsymbol{q}} m_{\boldsymbol{q}}-\sigma} \delta\left(\boldsymbol{k}_n - \sigma\boldsymbol{q} - \boldsymbol{k}_m\right), \quad (8)\end{aligned}$$

where $F\left(\boldsymbol{q}\right)$ is the e-p coupling function. Here the products are taken over all values of $\boldsymbol{q}'$ except $\boldsymbol{q}' = \boldsymbol{q}$.

Substituting Eqs. (6) and Eq.(8) in Eq.(4) and using the δ-function in Eq.(8) to perform integration over the electronic wavevector, we obtain for the second term in Eq.(4):

$$\begin{aligned}\Delta f_w\left(\boldsymbol{r}, \boldsymbol{p}, n_{\boldsymbol{q}}, n'_{\boldsymbol{q}}, t\right) = \frac{\hbar^3}{\left(2\pi\right)^3} \sum_{n,n'} e^{i\left(\boldsymbol{k}_n - \boldsymbol{k}_{n'}\right)\cdot\boldsymbol{r}} \delta^3\left(\boldsymbol{p} - \hbar\frac{\left(\boldsymbol{k}_n + \boldsymbol{k}_{n'}\right)}{2}\right) \int_{t_o}^{t} dt'\, e^{-i\frac{\hbar}{2m}\left(\boldsymbol{k}_n^2 - \boldsymbol{k}_{n'}^2\right)\left(t-t'\right)} \\ \times e^{-i\left(\omega\left(n_{\boldsymbol{q}}\right) - \omega\left(n'_{\boldsymbol{q}}\right)\right)\left(t-t'\right)} \sum_{m_{\boldsymbol{q}}} \int d\boldsymbol{r}' \int d\boldsymbol{p}' \sum_{\sigma=1,-1} \sum_{\boldsymbol{q}} F\left(\boldsymbol{q}\right) \\ \times \prod_{\boldsymbol{q}'\neq\boldsymbol{q}} \left\{ \sqrt{m_{\boldsymbol{q}} + \frac{1}{2}\left(1-\sigma\right)}\, \delta_{n_{\boldsymbol{q}'} m_{\boldsymbol{q}'}} \delta_{n_{\boldsymbol{q}} m_{\boldsymbol{q}}-\sigma} \right. \\ \times e^{-i\left(\boldsymbol{k}_n - \sigma\boldsymbol{q} - \boldsymbol{k}_{n'}\right)\cdot\boldsymbol{r}'} \delta^3\left(\boldsymbol{p}' - \hbar\frac{\left(\boldsymbol{k}_n - \sigma\boldsymbol{q} + \boldsymbol{k}_{n'}\right)}{2}\right) f_w\left(\boldsymbol{r}', \boldsymbol{p}', m_{\boldsymbol{q}}, n'_{\boldsymbol{q}}, t'\right) \\ - e^{-i\left(\boldsymbol{k}_n - \boldsymbol{k}_{n'} - \sigma\boldsymbol{q}\right)\cdot\boldsymbol{r}'} \delta^3\left(\boldsymbol{p}' - \hbar\frac{\left(\boldsymbol{k}_n + \boldsymbol{k}_{n'} + \sigma\boldsymbol{q}\right)}{2}\right) f_w\left(\boldsymbol{r}', \boldsymbol{p}', n_{\boldsymbol{q}}, m_{\boldsymbol{q}}, t'\right) \\ \left. \sqrt{m_{\boldsymbol{q}} + \frac{1}{2}\left(1+\sigma\right)}\, \delta_{m_{\boldsymbol{q}'} n'_{\boldsymbol{q}'}} \delta_{n'_{\boldsymbol{q}} m_{\boldsymbol{q}}+\sigma} \right\}. \quad (9)\end{aligned}$$

Performing integrations over electron coordinates and summing over the electronic states we get:

$$\Delta f_w\left(\boldsymbol{r},\boldsymbol{p},n_{\boldsymbol{q}},n'_{\boldsymbol{q}},t\right) = \int_{t_\circ}^{t} dt'\, e^{-i\left(\omega(n_{\boldsymbol{q}})-\omega\left(n'_{\boldsymbol{q}}\right)\right)(t-t')} \sum_{m_{\boldsymbol{q}}} \sum_{\sigma=1,-1} \sum_{\boldsymbol{q}} F\left(\boldsymbol{q}\right) e^{i\sigma\boldsymbol{q}\cdot\left(\boldsymbol{r}-\frac{\boldsymbol{p}}{m}(t-t')\right)}$$
$$\times \prod_{\boldsymbol{q}'\neq\boldsymbol{q}} \left\{ \sqrt{m_{\boldsymbol{q}}+\frac{1}{2}\left(1-\sigma\right)}\, \delta_{n_{\boldsymbol{q}'}m_{\boldsymbol{q}'}} \delta_{n_{\boldsymbol{q}}m_{\boldsymbol{q}}-\sigma} \right.$$
$$\times f_w\left(\boldsymbol{r}-\frac{\boldsymbol{p}}{m}\left(t-t'\right),\boldsymbol{p}-\sigma\frac{\hbar\boldsymbol{q}}{2},m_{\boldsymbol{q}},n'_{\boldsymbol{q}},t'\right)$$
$$-f_w\left(\boldsymbol{r}-\frac{\boldsymbol{p}}{m}\left(t-t'\right),\boldsymbol{p}+\sigma\frac{\hbar\boldsymbol{q}}{2},n_{\boldsymbol{q}},m_{\boldsymbol{q}},t'\right)$$
$$\left. \sqrt{m_{\boldsymbol{q}}+\frac{1}{2}\left(1+\sigma\right)}\, \delta_{m_{\boldsymbol{q}'}n'_{\boldsymbol{q}'}} \delta_{n'_{\boldsymbol{q}}m_{\boldsymbol{q}}+\sigma} \right\}. \qquad (10)$$

Substituting Eq.(10) into itself we obtain the second-order term corresponding to one scattering event. The second-order correction, e.g. for the terms corresponding to phonon emission, results to be

$$\Delta f_w\left(z,p_z,n_{\boldsymbol{q}},n_{\boldsymbol{q}},t\right) = 2\Re\Big\{ \sum_{\boldsymbol{q}} F^2\left(\boldsymbol{q}\right)\left\langle n_{\boldsymbol{q}}\right\rangle \int_{t_\circ}^{t} dt' \int_{t_\circ}^{t'} dt''\, e^{-i\boldsymbol{q}\cdot\frac{p_z+\hbar q/2}{m}(t'-t'')} e^{i\omega_{\boldsymbol{q}}(t'-t'')}$$
$$\times f_w\left(z-\tfrac{p_z}{m}\left(t-t'\right)-\tfrac{p_z+\hbar q/2}{m}\left(t'-t''\right)-\tfrac{p_z+\hbar q}{m}\left(t''-t_\circ\right),p_z+\hbar\boldsymbol{q},n_{\boldsymbol{q}}-1,n_{\boldsymbol{q}}-1,t_\circ\right)\Big\} \qquad (11)$$

The trajectories described by the above equation are represented in the diagrams contained in Fig. 1. They correspond to the semiclassical trajectories where $\boldsymbol{q}/2$ is transferred to the electron at each vertex. As a result of the time integrations, however, a sum over infinite trajectories gives the WF correction corresponding to a single scattering event.

IV. BOUNDARY CONDITIONS

Guided by the idea of Wigner trajectory introduced in the previous section, we face the problem of finding an equation equivalent to Eq. (4) for the WF in a finite region inside given boundaries. In fact, to solve the integral equation (4), we need to know the Wigner function at any given (z,p_z) at time $t_\circ$. Such initial condition is not suitable for describing an open system. In fact, by definition, a system is open when it can exchanges particles

with the environment: this means that there is a boundary between the system of interest and the rest of the universe. Therefore to model such a system the Wigner function has to be known at the initial time t_o inside the system and at all times on the boundary. From the analytical point of view this request corresponds to substituting in Eq. (4) the integral over the whole space by three terms. One term is identical to the original expression in Eq. (4), with the integral over the initial condition limited to the points internal to the device. The other two terms are evaluated at the two boundaries of the device. In the following we will derive the expression of this terms for the case in which the eigenstates of the unperturbed Hamiltonian are plain waves, considering, for the sake of simplicity, the one dimensional case. Under this assumption the coefficients of Eq. (5) can be rewritten as

$$\begin{aligned} f_{nn'}(z,p_z) &= \int dz'\, e^{-ip_z\cdot z'/\hbar} e^{ik_n\cdot(z+z'/2)} e^{-ik_{n'}\cdot(z-z'/2)} \\ &= e^{i(k_n-k_{n'})z}\delta\left(p_z-\hbar\frac{k_n+k_{n'}}{2}\right). \end{aligned} \tag{12}$$

Let us consider a device defined between $z=-A$ and $z=+A$. We will analyse now the ballistic term

$$\begin{aligned} f_w^{(o)l}\left(z,p_z,n_{\boldsymbol{q}},n'_{\boldsymbol{q}},t\right) &= \frac{1}{h}\sum_{nn'} f_{nn'}(z,p_z)\, e^{-i\left(\omega(nn_{\boldsymbol{q}})-\omega\left(n'n'_{\boldsymbol{q}}\right)\right)(t-t_o)} \int dz' \int dp'_z\, f^*_{nn'}(z',p'_z) \\ &\quad \times f_w\left(z',p'_z,n_{\boldsymbol{q}},n'_{\boldsymbol{q}},t_o\right). \end{aligned} \tag{13}$$

Substituting Eq. (12) in Eq. (13), considering at first $-\infty < z' < -A$, leads to

$$\begin{aligned} &f_w^{(o)l}\left(z,p_z,n_{\boldsymbol{q}},n'_{\boldsymbol{q}},t\right) \\ &= \frac{1}{h\,(2\pi)^2}\int dk_n \int dk_{n'}\, e^{i(k_n-k_{n'})z}\delta\left(p_z-\hbar\frac{k_n+k_{n'}}{2}\right) e^{-i(k_n-k_{n'})\frac{\hbar}{m}\frac{k_n+k_{n'}}{2}(t-t_o)} e^{-i\sum_{\boldsymbol{q}}\left(n_{\boldsymbol{q}}-n'_{\boldsymbol{q}}\right)\omega_{\boldsymbol{q}}(t-t_o)} \\ &\quad \times\frac{1}{h\,(2\pi)^2}\int dk_l \int dk_{l'} \int_{-\infty}^{-A} dz' \int dp'_z\, e^{-i(k_n-k_{n'})z'}\delta\left(p'_z-\hbar\frac{k_n+k_{n'}}{2}\right) e^{i(k_l-k_{l'})z'}\delta\left(p'_z-\hbar\frac{k_l+k_{l'}}{2}\right) \\ &\quad \times\int dz'' \int dp''_z\, e^{-i(k_l-k_{l'})z''}\delta\left(p''_z-\hbar\frac{k_l+k_{l'}}{2}\right) f_w\left(z'',p''_z,n_{\boldsymbol{q}},n'_{\boldsymbol{q}},t_o\right). \end{aligned} \tag{14}$$

From the properties of the δ-function we get

$$z' < -A \Rightarrow z - \frac{p'_z}{m}(t - t_\circ) < -A \Rightarrow \begin{cases} t > t_\circ + \frac{z-(-A)}{\frac{p'_z}{m}}, \text{if } p'_z > 0 \\ \\ t < t_\circ + \frac{z-(-A)}{\frac{p'_z}{m}}, \text{if } p'_z < 0 \end{cases} \tag{15}$$

Since in this specific case, particle entering the device from the left boundary, the condition $p'_z < 0$ can not be verified, we are left with

$$t_\circ < t - \frac{z-(-A)}{\frac{p'_z}{m}} < t, \text{if } p'_z > 0. \tag{16}$$

Setting

$$\tau = t - \frac{z-(-A)}{\frac{p'_z}{m}} = t - \frac{z' + \frac{p'_z}{m}(t - t_\circ) - (-A)}{\frac{p'_z}{m}} = t_\circ - \frac{z' - (-A)}{\frac{p'_z}{m}} \tag{17}$$

yields

$$z' = -A - \frac{p'_z}{m}(\tau - t_\circ). \tag{18}$$

Then we can perform a change of coordinates from (z', p'_z) to (τ, ξ) as follows:

$$\begin{cases} z' = -A - \frac{\xi}{m}(\tau - t_\circ), \ t_\circ < \tau < t \\ \\ p'_z = \xi \qquad\qquad , \ \xi > 0 \end{cases} ; \qquad \det J = \det \begin{pmatrix} -\frac{\xi}{m} - \frac{1}{m}(\tau - t_\circ) & \\ \\ 0 & 1 \end{pmatrix} = -\frac{\xi}{m} \tag{19}$$

obtaining in conclusion:

$$\begin{aligned} f_w^{(\circ)l}\left(z, p_z, n_{\boldsymbol{q}}, n'_{\boldsymbol{q}}, t\right) &= \int_{t_\circ}^{t} dt' \int_0^{+\infty} dp'_z \frac{p'_z}{m} h \sum_{nn'} f_{nn'}(z, p_z)\, e^{-i\left(\omega(nn_{\boldsymbol{q}}) - \omega\left(n'n'_{\boldsymbol{q}}\right)\right)(t-t')} f^*_{nn'}(-A, p'_z) \\ &\quad \times \frac{1}{h} \sum_{ll'} f_{ll'}(-A, p'_z)\, e^{-i\left(\omega(ln_{\boldsymbol{q}}) - \omega\left(l'n'_{\boldsymbol{q}}\right)\right)(t'-t_\circ)} \\ &\quad \times \int dz'' \int dp''_z\, f^*_{ll'}(z'', p''_z)\, f_w\left(z'', p''_z, n_{\boldsymbol{q}}, n'_{\boldsymbol{q}}, t_\circ\right) \\ &= \frac{1}{h} \sum_{nn'} f_{nn'}(z, p_z) \int_{t_\circ}^{t} dt'\, e^{-i\left(\omega(nn_{\boldsymbol{q}}) - \omega\left(n'n'_{\boldsymbol{q}}\right)\right)(t-t')} \\ &\quad \times \int_0^{+\infty} dp_z^{prime} \frac{p'_z}{m} f^*_{nn'}(-A, p'_z)\, f_w\left(-A, p'_z, n_{\boldsymbol{q}}, n'_{\boldsymbol{q}}, t'\right). \end{aligned} \tag{20}$$

The same procedure can be applied in the case $+A < z' < +\infty$.

The details of the derivation for the terms including scattering events require a more sophisticated analysis and are discussed in Ref. [7]. Here we simply report the final result:

$$
\begin{aligned}
& f_w\left(z, p_z, n_q, n'_q, t\right) = \\
& \frac{1}{h}\sum_{nn'} f_{nn'}\left(z, p_z\right) e^{-i\left(\omega(nn_q)-\omega\left(n'n'_q\right)\right)(t-t_\circ)} \int_{-A}^{A} dz' \int dp'_z f^*_{nn'}\left(z', p'_z\right) f_w\left(z', p'_z, n_q, n'_q, t_\circ\right) \\
& + \frac{1}{h}\sum_{nn'} f_{nn'}\left(z, p_z\right) \int_{t_\circ}^{t} dt' \, e^{-i\left(\omega(nn_q)-\omega\left(n'n'_q\right)\right)(t-t')} \Bigg\{ \Bigg[\int_0^{+\infty} dp'_z \frac{p'_z}{m} f^*_{nn'}\left(-A, p'_z\right) \\
& \times f_w\left(-A, p'_z, n_q, n'_q, t'\right) - \int_{-\infty}^{0} dp'_z \frac{p'_z}{m} f^*_{nn'}\left(A, p'_z\right) f_w\left(A, p'_z, n_q, n'_q, t'\right) \Bigg] \\
& + \int_{-A}^{A} dz' \int dp'_z \sum_{mm_q} \Big[\mathcal{H}'\left(nn_q, mm_q\right) f^*_{mn'}\left(z', p'_z\right) f_w\left(z', p'_z, m_q, n'_q, t'\right) \\
& - f^*_{nm}\left(z', p'_z\right) f_w\left(z', p'_z, n_q, m_q, t'\right) \mathcal{H}'\left(mm_q, n'n'_q\right) \Big] \Bigg\}. \qquad (21)
\end{aligned}
$$

where again for simplicity a one-dimensional case has been considered, and $-A$ and A are the device boundaries.

In order to verify the correctness of the use of the boundary conditions for an open mesoscopic system we have first evaluated the ballistic evolution of the first term in Eq. (21) assuming a step potential profile, $f_w = 0$ at $t = t_\circ$ inside the device, and a Maxwellian local-equilibrium incoming distribution at the left and right boundaries. Results are shown in Fig. 2 at different times after the initial condition.

At the longest times we recover for f_w the same result which is obtained without using boundary conditions for a stationary infinite system, where f_w is evaluated by means of an equilibrium density matrix diagonal over the scattering states.

V. APPLICATIONS

In order to evaluate the effect of an e-p scattering event on the WF we have performed an iterative expansion of Eq. (21) up to the second order in the e-p perturbation Hamiltonian. As a case of study we have considered a step potential profile. Integrations in time have been performed analytically; the integrals over z', p'_z and over the electron states have been

evaluated with full numerical integration while the integral over the phonon modes has been performed by means of a Monte Carlo selection. Space correlations for the evaluation of the coefficients in Eq. (5) have been considered up to 40 nm. The steady-state WF for a 0.1 eV step including the effect of an e-p scattering event is presented in Fig. 3. Fig. 4 shows the current as a function of the step potential as obtained with the ballistic WF (solid curve) and with the WF corrected by the effect of an e-p scattering process (circles) switched on 50 fs before the "observation time". Comparison is presented with the outcomes of a semiclassical calculation based on the Boltzmann equation. The quantum ballistic curve is always lower then the corresponding semiclassical one, and instead of reaching a saturation value, rise up to a maximum and then decreases. This is due to the fact that in the quantum picture increasing the potential step leads, as a consequence of quantum reflection, to a decrease of the transmission coefficient that is to a decrease of the current intensity. Finally, in both quantum and semiclassical calculations the effect of the e-p interaction is, as expected, a reduction of the current with respect to the ballistic case.

VI. COHERENT TRANSPORT IN MESOSCOPIC DEVICES

Concerning the study of coherent phenomena in open-boundary 2D systems, during this last year, the research activity has proceeded both from the theoretical and the application standpoints.

As for the first one, the inclusion of the magnetic field inside the numerical solver of the 2D Schrödinger equation has been achieved. This has allowed to investigate, for example, the role of the magnetic field on the conductance of rough quantum wells [8]. While the conductance of an ideal quantum well is greately deteriorated by the roughness present at its surface, the presence of a magnetic field partly recovers it. The magnetic field modifies the coherent behaviour of electrons leading to conduction properties that depend on its strength [9].

We have analized a rough quantum wire, where the roughness is modelled with a gaussian

autocorrelation and the potential is zero inside the channel and infinity at the boundary. In a rough quantum wire the magnetic field reduce the effect of roughness increasing the conductance.

Fig. 5a shows the squared modulus of the electron wave-function for the case of an electron in a rough channel. The carrier is in the fundamental subband, since it is supposed to have total energy lower than the threshold of the first-excited subband, and is coming from the left side of the channel. Getting close to the right boundary, since the channel becomes wider, the electron moves into the upper subband. This produces a reflection of the electron, and decreases the conductance. In presence of a magnetic field the electron approaches one of the edge of the channel (Fig. 5b: positive magnetic field; Fig. 5c: same value of the field as in Fig. 5b, but with negative sign) and the backscattering is strongly reduced. The two situations shown in Fig.s 5b-5c are equivalent from the transport standpoint. In fact, because of the Onsager relation, that is a consequence of the time inversion symmetry, the conductance depends only on the absolute value of the magnetic field not on its sign.

The effect of the magnetic field on the conduction properties of rough channel is indepen-det from the roughness. This can be seen studing a large ensamble of rough channels with different roughness. In Fig. 6 it is shown the distribution of the conductance values over the samples, at increasing magnetic field. The trasversal region in wich the electron is costrained by the magnetic field is well indicated by the magnetic length $l_B = \sqrt{\hbar/|eB|}$, where B is the value of the magnetic field. The label L-inf in the first graph of Fig. 6 indicates the zero magnetic field case, in the other two graphs the magnetic field increases, and the magnetic length l_B takes the values L/2 and L/4, where L is the mean width of the channel. The conductance distribution at zero magnetic field shows a tail at low conductance values that is progressively reduced by increasing the magnetic field.

On the application side, the effect of channel quantization in silicon MOSFET has been investigated. In particular, different devices, which are considered possible alternatives to standard MOSFETs for the next ULSI generations, have been explored. In [10], [11] threshold voltage shift, capacitance reduction, and mobility enhancement have been studied

for highly non-homogeneous devices. In these devices, a low-doping layer is epitaxially grown on a standard high-doping substrate. As can be seen in [10], [11], the presence of the epi-layer doesn't degrade the capacitance of the MOS while mobility is improved by the use of low dopings. In addition, short channel effects are still under control through the buried high doping layer.

The same kind of investigation has also been performed on single- and double-gate MOS devices [12], [13]. In particular, the relevance of the so called volume inversion due to size quantization, as opposed to the reduction of transverse effective field, in improving the electron low-field mobility in such devices has been explored.

VII. CONCLUSIONS

In this final report we have presented the main results achieved under this contract.

A theoretical and computational analysis of the quantum dynamics of charge carriers in presence of electron-phonon interaction based on the Wigner function has been applied to the study of transport in mesoscopic systems.

We have shown the existence of Wigner trajectories both for the ballistic evolution of the WF and for the case in which e-p scattering is included.

We have faced the problem of finding an equation for the WF in a finite region inside given boundaries. We have proved that for the solution of the integral equation describing the WF it is possible to substitute the knowledge of the WF over all space at a given (initial) time t_o with the knowledge of the same function inside the region of interest at t_o and at all times at the boundary for "entering" momenta.

From the application standpoint we have analyzed the effect of an e-p scattering event on the WF for the case of a step potential profile. Results for the current in comparison with semiclassical calculations are presented.

Concerning the study of coherent phenomena in open-boundary 2D systems, the inclusion of the magnetic field inside the numerical solver of the 2D Schrödinger equation has been

achieved. This has allowed to investigate the role of the magnetic field on the condactance of rough quantum wells. It is found that in both structures the magnetic field reduce the effect of roughness increasing the conductance.

Finally the effect of channel quantization in silicon MOSFETs has been investigated. In particular, different devices which are considered possible alternatives to standard MOSFETs for the next ULSI generations, have been explored.

VIII. PUBLICATIONS

- C. Fiegna, A. Abramo, "Optimization of channel profiles for ultra-short MOSFETs by quantum simulation", in *IEDM Tech. Digest*, 815, S. Francisco, CA (USA), Dec. 1996.

- A. Abramo, "A general purpose 2D Schrödinger solver with open/closed boundary conditions for quantum device analysis", in *SISPAD Tech. Digest*, p. 105, Boston, MA (USA), Sep. 1997.

- C. Fiegna, A. Abramo, "Solution of 1-D Schrödinger and Poisson equations in single and double gate SOI MOS", in *SISPAD Tech. Digest*, p. 93, Boston, MA (USA), Sep. 1997.

- M. Nedjalkov, I. Dimov, P. Bordone, R. Brunetti and C. Jacoboni "Using the Wigner Function for Quantum Transport in Device Simulation", Mathl. and Comput. Modelling **25**, 33 (1997).

- C. Fiegna, A. Abramo, "Analysis of quantum effects in non-uniformly doped MOS structure", in press on *IEEE Transaction Electron Devices.*

- C. Jacoboni, A. Abramo, P. Bordone, R. Brunetti, and M. Pascoli "Application of the Wigner-Function Formulation to Mesoscopic Systems in Presence of Electron-Phonon Interaction" accepted for publication on *VLSI Design.*

- P. Bordone, A. Abramo, R. Brunetti, M. Pascoli and C. Jacoboni "Wigner Function for Open Systems with Electron-Phonon Interaction", accepted for publication on Physica Status Solidi.

- R. Brunetti and C. Jacoboni "Wave-packet analysis of electron-phonon interaction in the Wigner formalism", accepted for publication on Phys. Rev. B

- C. Fiegna, A. Abramo, "One-dimensional quantum simulation of single- and double-gate MOS structures", submitted to *IEEE Transaction Electron Devices.*

- M. Pascoli, P. Bordone, R. Brunetti, and C. Jacoboni, *Wigner trajectories for electrons interacting with phonons*, in preparation.

A copy of each of the above publication is enclosed.

REFERENCES

[1] W.R. Frensley,*Boundary conditions for open quantum systems driven far from equilibrium*, Rev. Mod. Phys. **62**, 745 (1990).

[2] W.R. Frensley, *Wigner-function model of a resonant-tunneling semiconductor device*, Phys. Rev. B**36**, 1570 (1987).

[3] N.C. Kluksdahl, A.M. Kriman, D.K. Ferry, and C. Ringhofer, *Self-consistent study of the resonant tunneling diode*, Phys. Rev. B**39**, 7720 (1989).

[4] W.R. Frensley, *Quantum transport modeling of resonant-tunneling devices*, Solid State Electron. **31**, 739 (1988).

[5] F. Rossi, C. Jacoboni, and M. Nedjalkov, *A Monte Carlo solution of the Wigner transport equation*, Semicond. Sci. Technol. **9**, 934 (1994).

[6] R. Brunetti, C. Jacoboni, and F. Rossi, *Quantum theory of transient transport in semiconductors: a Monte Carlo approach*, Phys. Rev. B**39**, 10781 (1989).

[7] C. Jacoboni, A. Abramo, P. Bordone, R. Brunetti, and M. Pascoli, *A generalized Wigner function approach to quantum transport in mesoscopic systems*, in preparation.

[8] A. Abramo, *A general purpose 2D Schrödinger solver with open/closed boundary conditions for quantum device analysis*, in *SISPAD Tech. Digest*, p. 105, Boston, MA (USA), Sep. 1997.

[9] R.A. Webb, S. Washburn, C.P. Umbach, and R.B. Laibowitz, Phys. Rev. Lett. **54**, 2696 (1985).

[10] C. Fiegna, A. Abramo, *Optimization of channel profiles for ultra-short MOSFETs by quantum simulation*, in *IEDM Tech. Digest*, 815, S. Francisco, CA (USA), Dec. 1996.

[11] C. Fiegna, A. Abramo, *Analysis of quantum effects in non-uniformly doped MOS structure*, in press on *IEEE Transaction Electron Devices.*

[12] C. Fiegna, A. Abramo, *Solution of 1-D Schrödinger and Poisson equations in single and double gate SOI MOS*, in *SISPAD Tech. Digest*, p. 93, Boston, MA (USA), Sep. 1997.

[13] C. Fiegna, A. Abramo, *One-dimensional quantum simulation of single- and double-gate MOS structures*, submitted to *IEEE Transaction Electron Devices.*

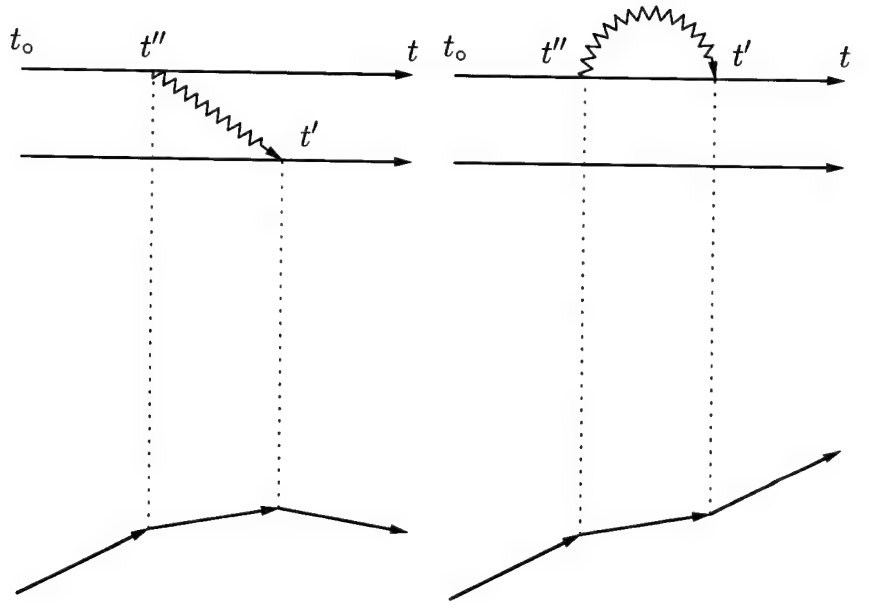

Fig.1 Example of the Wigner trajectories that contribute to the result in Eq. (4) for real and virtual emissions of a mode q.

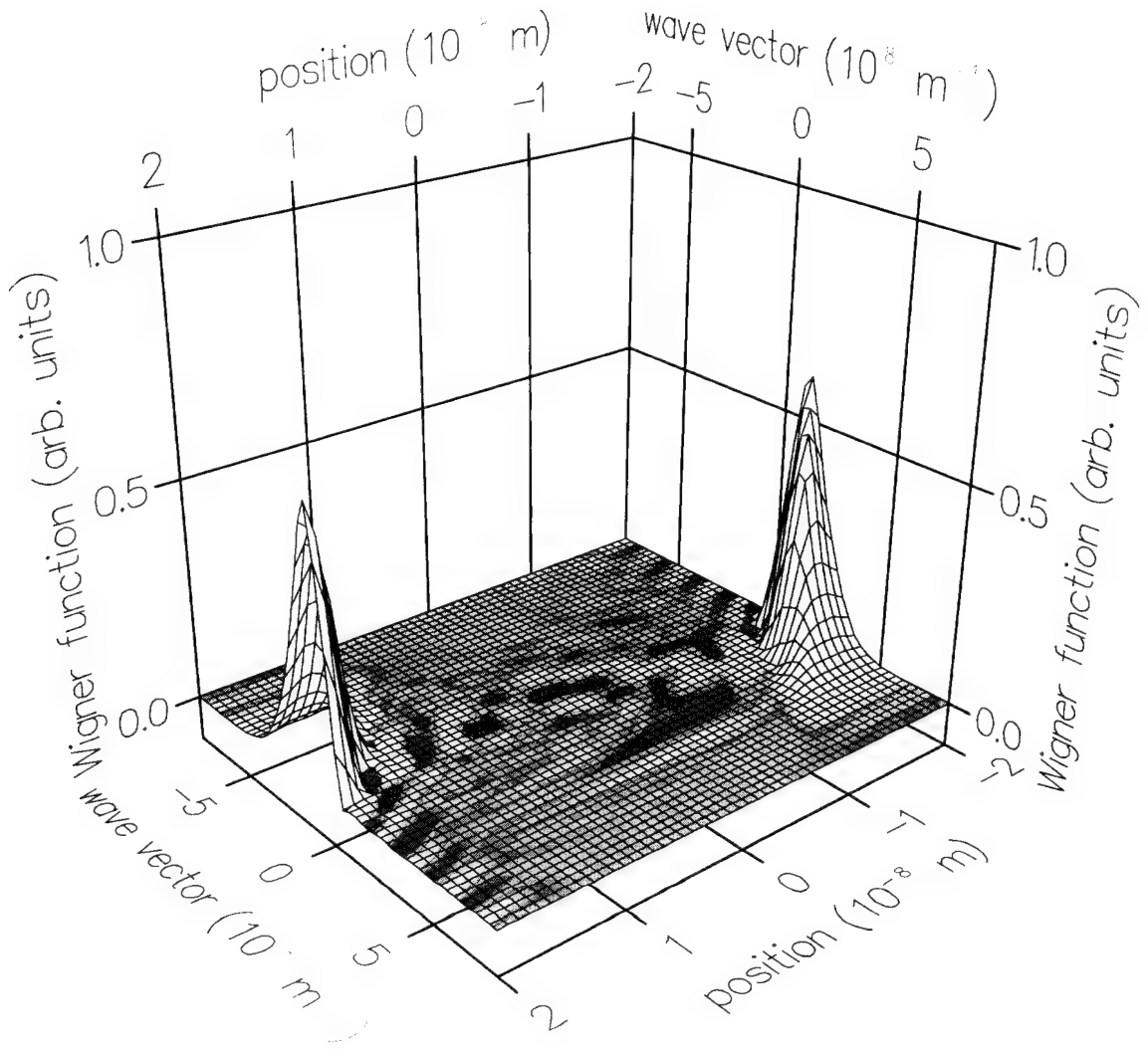

Fig.2a Ballistic evolution of the first term in Eq. (21) at $t = 10$ fs for electrons entering from the boundaries into a region with a potential step.

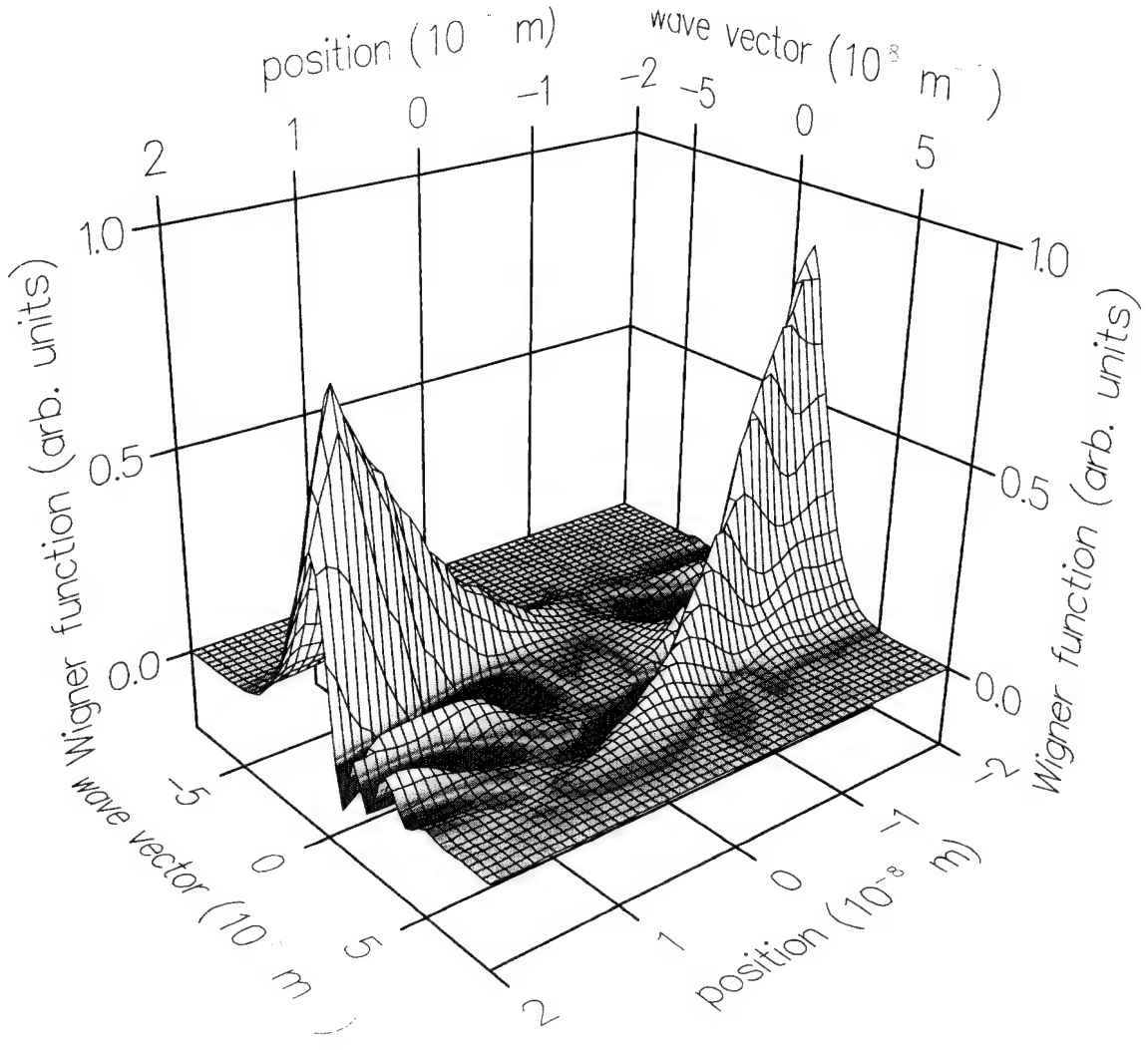

Fig.2b Same as in Fig. 2a) at $t = 40$ fs.

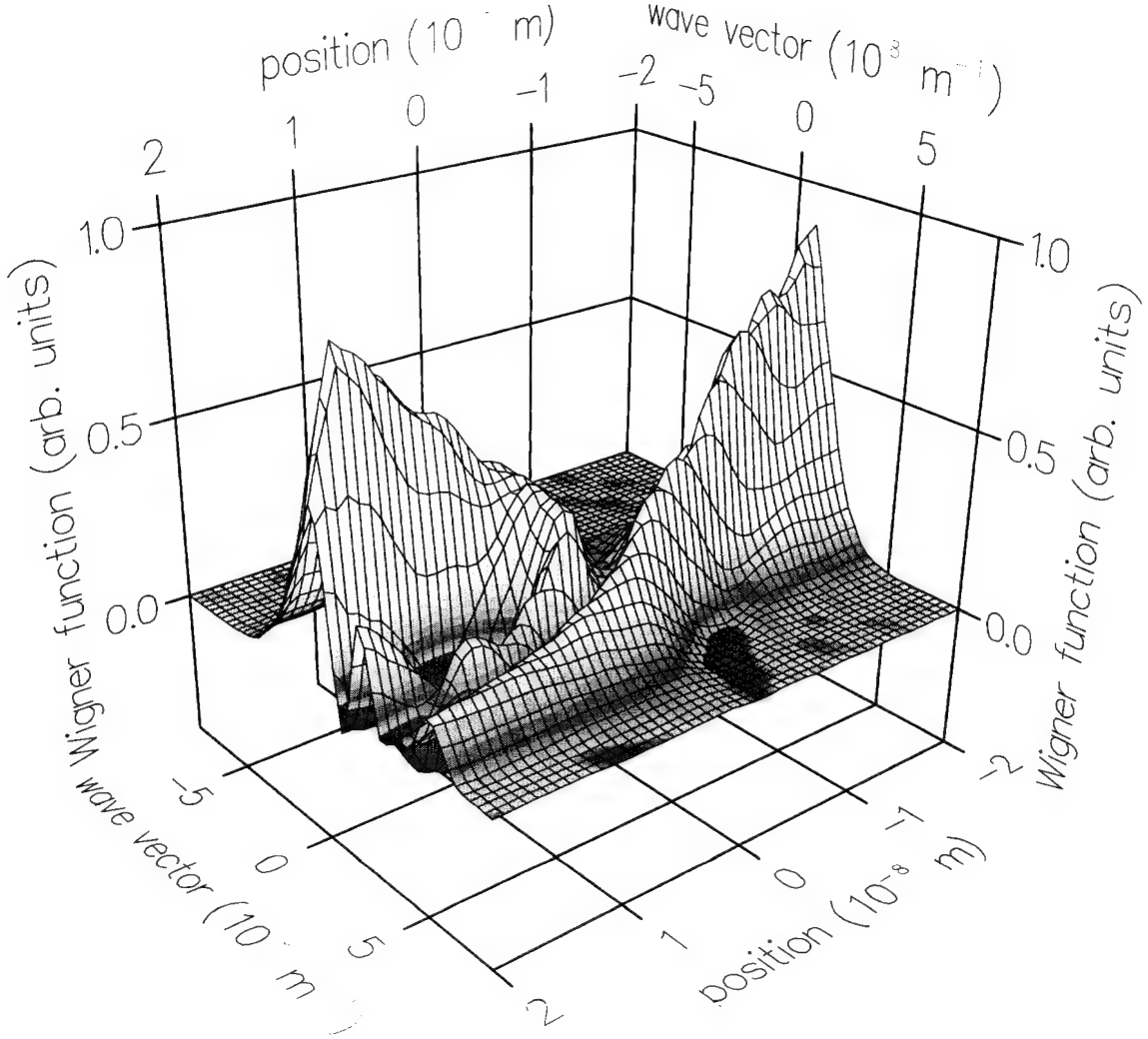

Fig.2c Same as in Fig. 2a) at $t = 80$ fs.

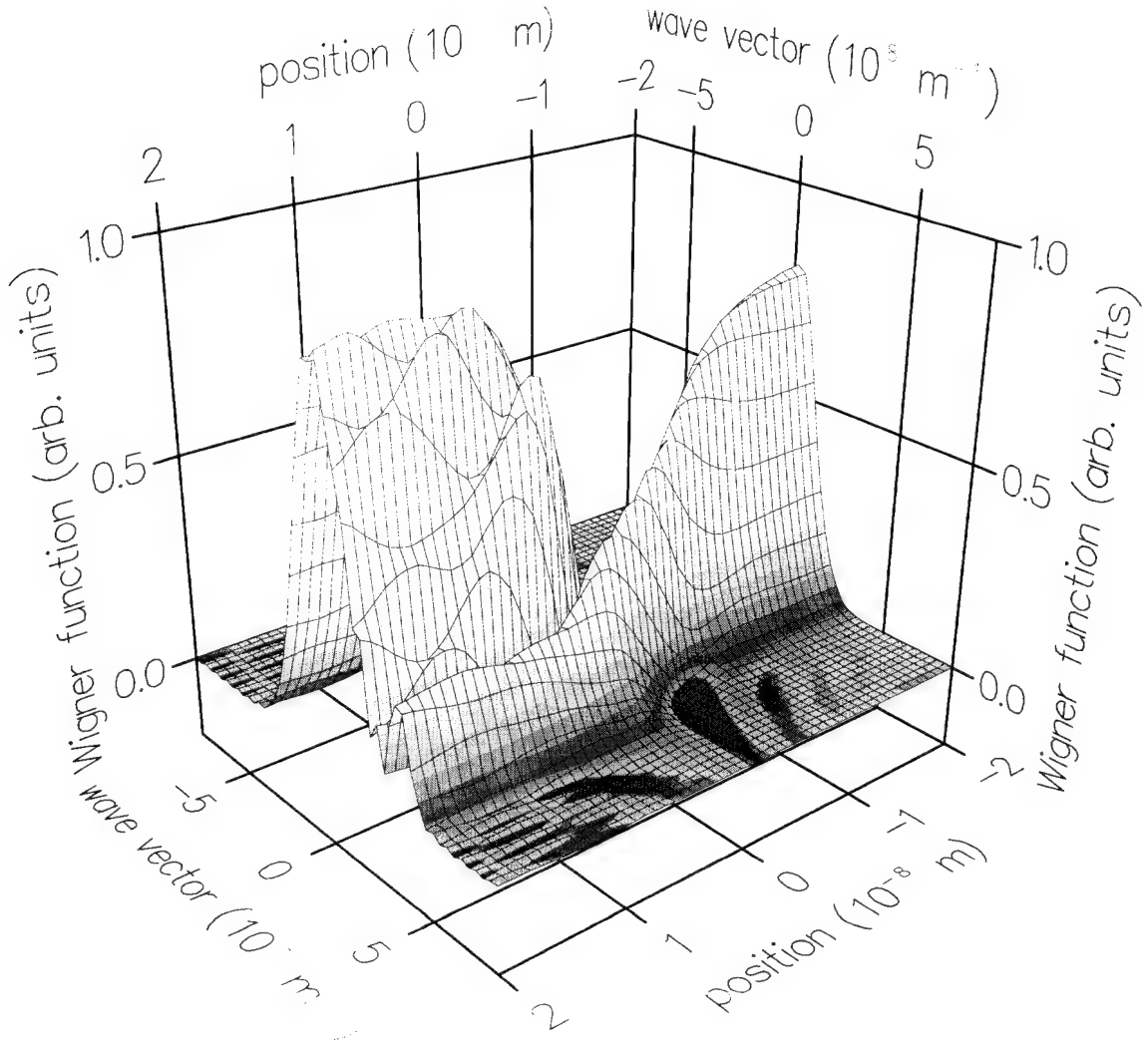

Fig.2d Stationary Wigner function for a 0.1 eV potential step, as obtained by means of an equilibrium density matrix diagonal over the scattering states.

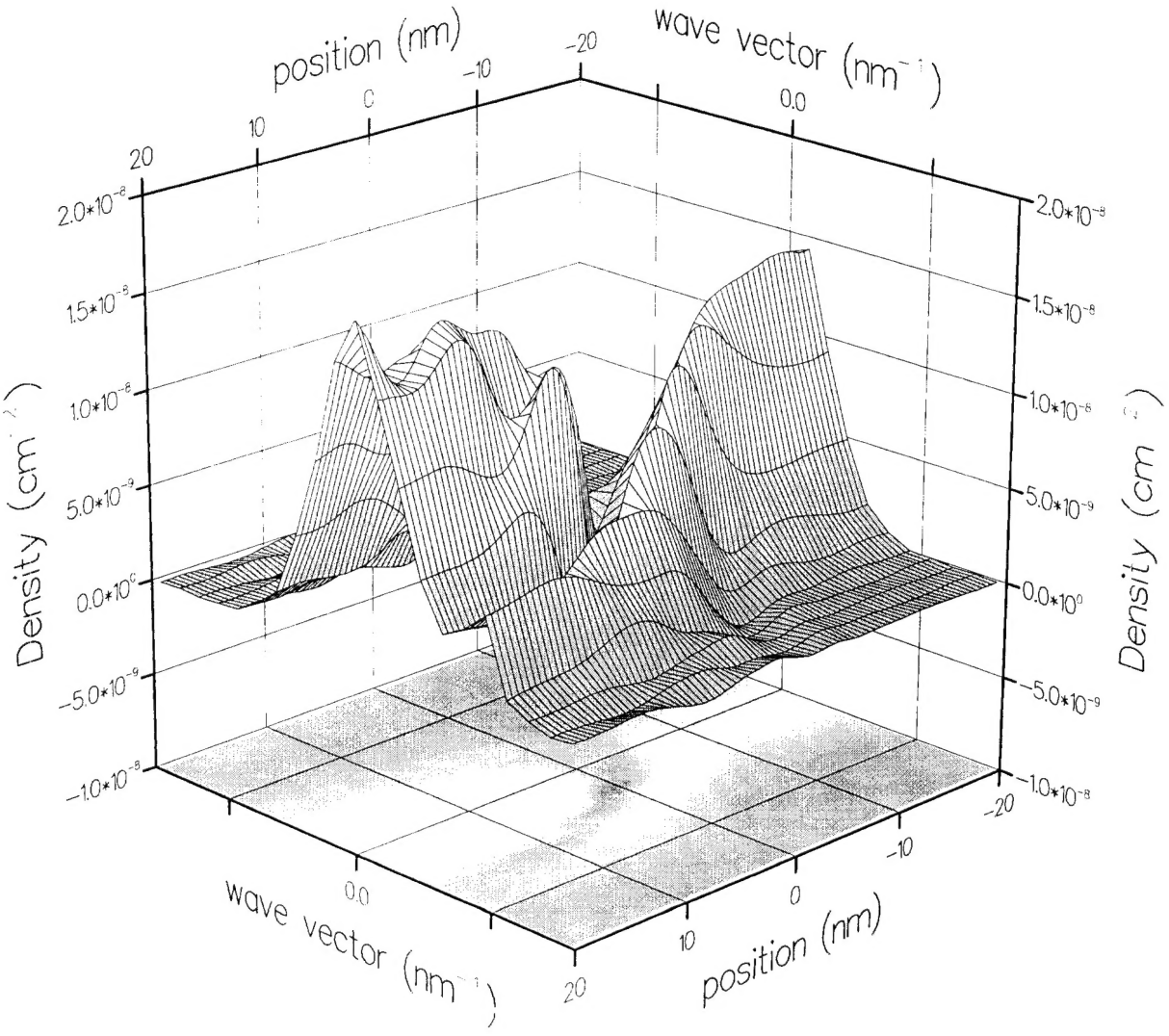

Fig.3 Wigner function for a 0.1 eV potential step, including the effect of an e-p scattering switched on 50 fs before the "observation" time.

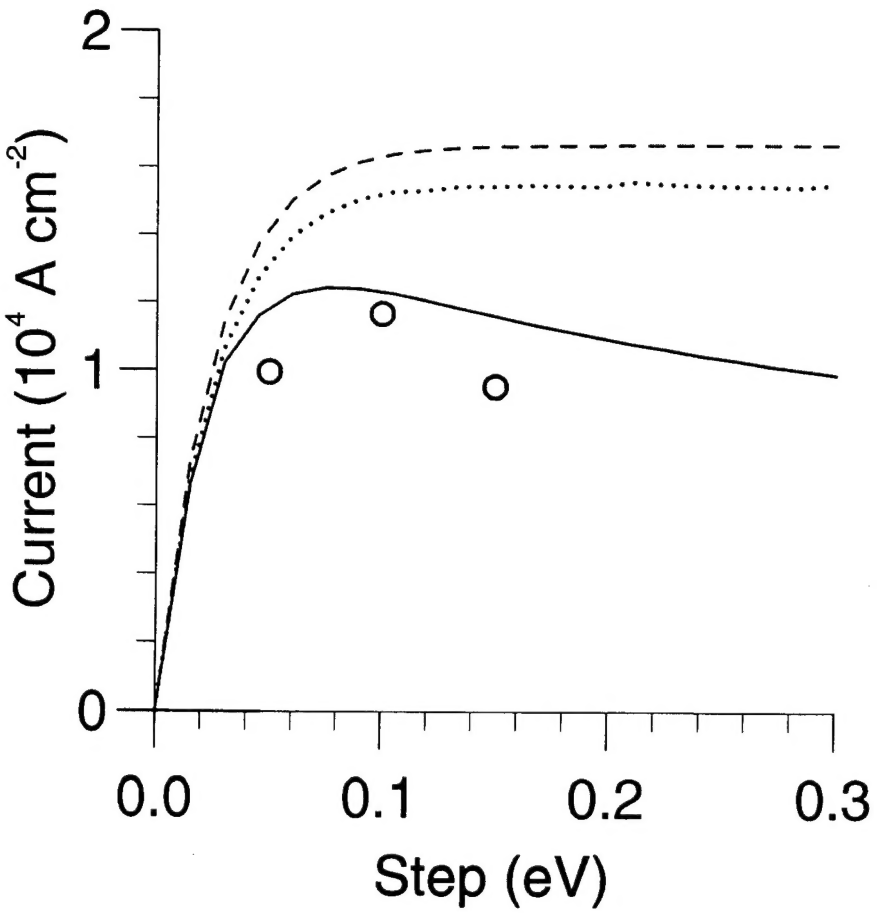

Fig.4 Current as a function of the step potential. Comparison between quantum and semiclassical calculations with and without e-p interaction. Wigner ballistic curve (solid line), Wigner curve with e-p scattering (circles), semiclassical ballistic curve (dashed line), semiclassical curve with e-p scattering (dotted line). Carrier density at the contacts $n = 10^{16}$ cm^{-3}.

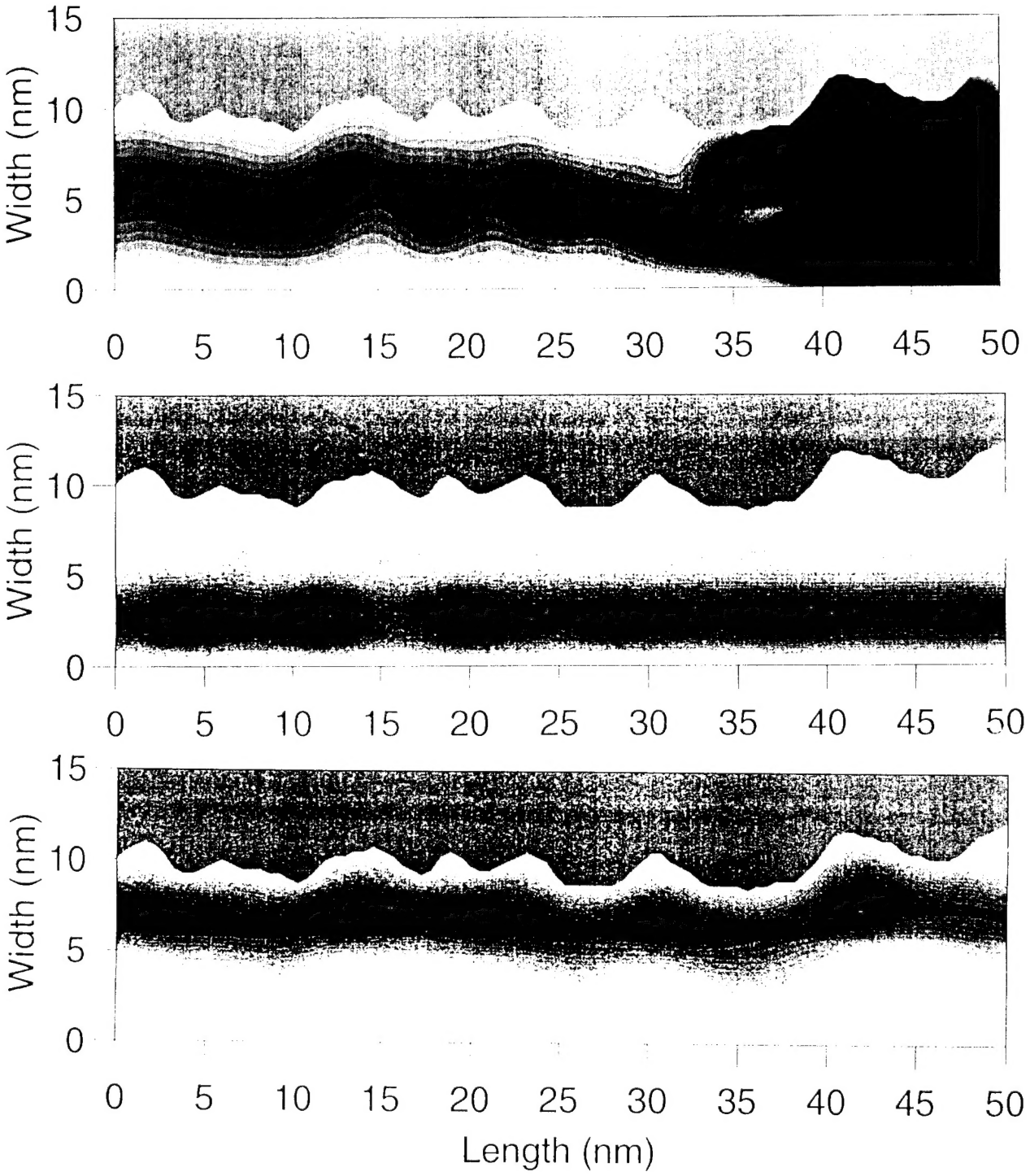

Fig.5 Squared modulus of the electron wave-function in a rough channel for the case of a carrier in the fundamental subband having total energy lower then the threshold of the first excited subband and coming from the left. a) No magnetic field; b) positive magnetic field; c) nagative magnetic field with the same value as in b).

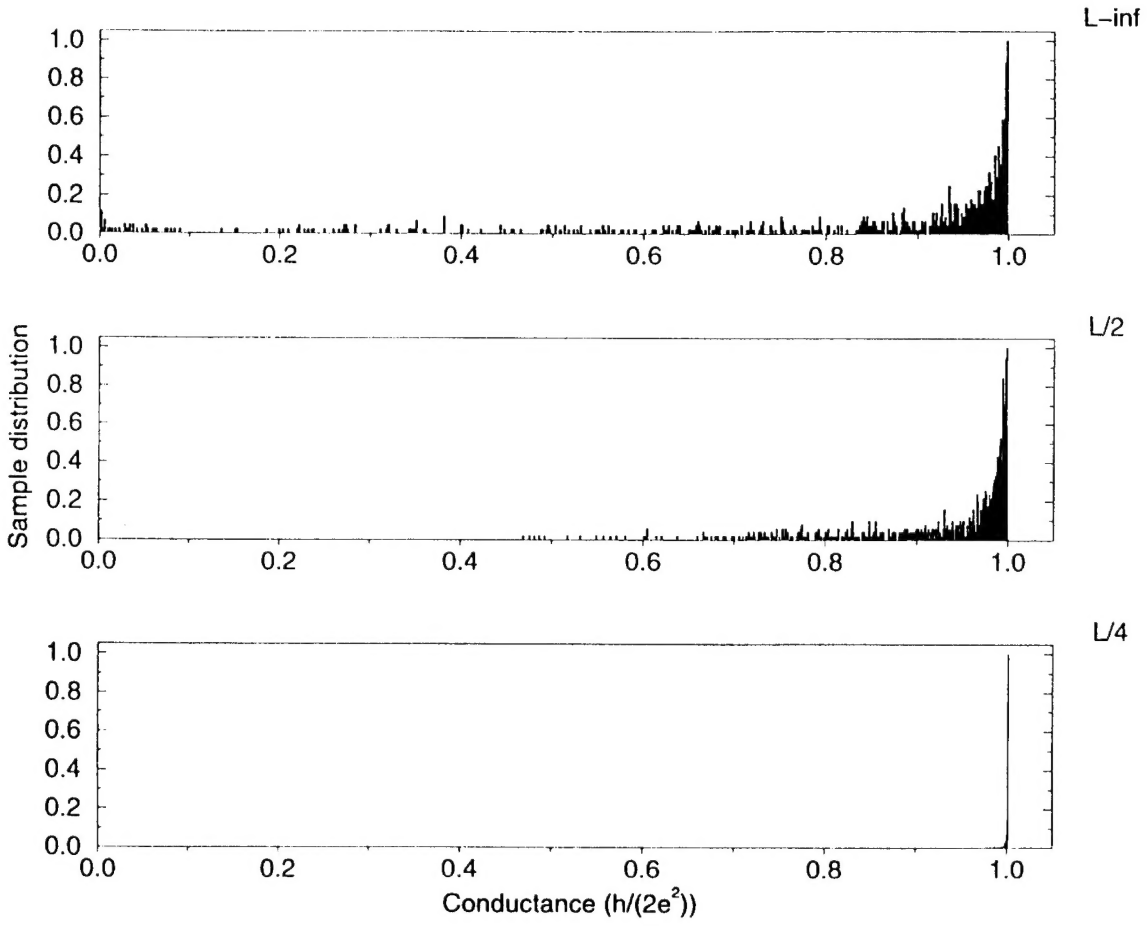

Fig.6 Distribution of the conductance values over an ensamble of samples, at increasing magnetic fields, normalized to the peak value (see the text for the meaning of the symbols).